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**Unoccupied Electronic States in MgCNi<sub>3</sub> Superconductor: an Ni K- and Ni L<sub>3</sub>- Edge Studies**

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Beamline(s): X18B, X11A

**Introduction:** Newly discovered MgCNi<sub>3</sub> superconductor showed lower than cubic *Pm-3m* symmetry of Ni<sub>6</sub> octahedra [1]. The local distortions are often viewed as a signature of local charge density waves (LCDWs) and/or local spin density waves (LSDWs). This work is undertaken to explore an impact of onset of LCDWs and LSDWs upon the unoccupied electronic states probed by Ni K- and Ni L<sub>3</sub>- edge x-ray absorption near edge structure (XANES).

**Methods and Materials:** We performed high resolution Ni K-edge XANES measurements of MgCNi<sub>3</sub> in a temperature range of 3-300K. Measurements were done at beamlines X18B and X11A in transmission mode.

**Results:** The experimental spectra become slightly broader with increasing temperature showing no anomalies or crossovers neither in vicinity of  $T_c \sim 7$  K nor between 50 and 200 K (where transport, NMR, and EXAFS measurements indicate the crossover behavior presumably due to the onset of LCDWs and/or LSDWs) [1]. All features at the Ni K-edge can be understood in terms of single-electron multiple scattering (MS) calculations for large clusters of atoms. Direct simulations indicate that these features exhibit very weak response upon *local* displacements of Ni atoms ( $\leq 0.06$  Å) from their original position in the cubic *Pm-3m* lattice in combination with *local* magnetic moments at Ni site ( $\leq 0.9\mu_B$ ). The Ni K-edge XANES results illustrate that Ni *p*-like states have a little, if any, impact upon the electronic properties of MgCNi<sub>3</sub>.

Contrary, the Ni L<sub>3</sub>-edge MS simulations show a high sensitivity of the L<sub>3</sub>- edge profile to the local displacements and/or the local magnetic moments at the Ni site revealing several changes that could be observed experimentally. Temperature-dependent Ni L<sub>3</sub>-edge XANES/XMCD measurements need to be done to adjust the parameters of our models.

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**References:** [1] A.Yu. Ignatov, L.M. Dieng, T.A. Tyson, T. He, and R.J. Cava, "Observation of a low symmetry crystal structure for superconducting MgCNi<sub>3</sub> by Ni K- Edge x-ray absorption measurements", (Submitted to Phys. Rev. B).